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Characterization of a Gas/Gas, Hydrogen/Oxygen Engine

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CHARACTERIZATION OF A GAS/GAS, HYDROGEN/OXYGEN ENGINE

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Abstract

As part of an ongoing program to develop a computational methodology to obtain high-fidelity rocket engine flow solutions, computations were performed on a single-element, gas/gas, H_2/O_2 combustion engine. The present work examines the influence of modeling experimental features often neglected in a simulation, specifically a nitrogen curtain purge used to cool optical access. It is shown that the influence is significant and better agreement with the data can be obtained by including the nitrogen purge. Additional solutions are presented to investigate the impact of using various turbulence models on this class of problems. A linear, realizable k-epsilon model best represented the experimental data, however, it should be recognized that RANS-type turbulence models are best suited to steady, isotropic flows, which the present flowfield is not.

Introduction

Staged combustion cycle engines, such as the H_2/O_2 Integrated Powerhead Demo or a staged combustion hydrocarbon boost engine, have become a focus of research within the rocket propulsion community. In support of this research, ongoing computational and experimental efforts have advanced the development of a design methodology for gas/gas injectors. The goal is to use experimental measurements to anchor state-of-the-art codes which can then be used to investigate a series of injector configurations. This provides a more efficient design process, resulting in significant savings in full-scale development time and costs.

This paper focuses on continuing efforts to develop a computational methodology to efficiently, accurately, and robustly obtain high-fidelity solutions of combusting rocket engines so as to gain a knowledge and understanding of their features. Simulations of a combusting, single-element, shear-coaxial, H_2/O_2 engine were performed to characterize its flowfield and investigate a set of turbulence models to determine which might be most suitable to this class of problems. In addition, averaged transient solutions are examined to provide an analysis of the sensitivity to the solutions when features unique to an experimental setup are neglected in a simulation. Experimental data are shown for comparison to help illustrate the conclusions.

This class of problems has been previously investigated both experimentally[1,2] and computationally.[2,3,4,5] The experiments produced data on hydrogen and oxygen mole fractions, mean and RMS velocities, and OH-radical concentration. This problem has since been used as a benchmark for assessing CFD capabilities for designing gas/gas injectors within a rocket combustor environment. Recent computational investigations[5] showed that solutions could be achieved on finer grids than previously reported[2,4] using a second-order, implicit, upwind, preconditioning scheme. These solutions compare well with experiment and reveal additional

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structure near the injectors. It was also shown in Reference 5 that a time-averaged transient solution produces a different result than does a "quasi-steady" solution due to the inherently unsteady nature of coaxial shear flows.

In the present study, the authors examine the effects of a nitrogen purge (used in the experiment to cool the optical access) to determine its effects on the flow near the center of the engine. While often neglected in many computational models, it will be shown that such experimental features do impact the flow, biasing the data. Additionally, the influence of various turbulence models, including, a linear, realizable k-epsilon,[6] cubic k-epsilon,[7] one-equation Goldberg R_t,[8] and k-epsilon-R_t[9] are investigated to determine which may be most suitable to this class of problems.

Computational Model

Calculations were performed using the CFD++ flow solver from Metacomp Technologies, Inc.[10,11] The code has the capability to solve the Reynolds-Averaged Navier-Stokes (RANS) equations, the Large Eddy Simulation (LES) equations, or a RANS/LES hybrid set of equations on 3-D structured and unstructured grids. It is a compressible/incompressible flow code with high- and low-speed capability and has both finite-rate and equilibrium chemistry options. Low-speed flows are solved using a preconditioning algorithm. Explicit (Runge-Kutta) and implicit schemes are available for both steady and unsteady flows.

For the present problem, hydrogen gas flows through an annulus surrounding a central core of gaseous oxygen. The gases enter the combustion chamber where they mix in a shear layer and react. The experimental hardware has a converging section at the end of the chamber which terminates at the throat where the gas is expelled to the atmosphere. In the computational setup, however, this section has been omitted to be consistent with previous calculations.[5]

Oxygen was injected into the chamber at a mass flow rate of 0.042 kg/s (0.1 lbm/sec) with an O/F ratio of 4. The chamber pressure was specified at 1.29 MPa and the inlet temperature at 297K. The injectors were modeled sufficiently upstream so that a fully-developed turbulent profile has formed by the time the gas enters the chamber. Standard non-reflecting, subsonic boundary conditions were imposed at the outflow boundary, as well as no-slip conditions at solid surfaces and a symmetry condition on the centerline. All the two-dimensional calculations were done by assuming the flow to be axisymmetric, including the effects of a nitrogen purge used in the experiment to cool the optical access.

Eight processors of an SGI Origins 3800 computer ran the simulations at the Edwards Distributed Computing Center. CFD++ was set up to run the 2-D axisymmetric, compressible, real gas equations, discretized with a second-order, upwind finite-volume scheme on a grid consisting of 53740 cells. Stretching the grid resolved the region near the injectors and provided an adequate number of grid cells within the boundary layer inside the injectors. The time-accurate calculations were carried out using an implicit, preconditioned, dual time stepping algorithm. Combustion was handled using the Anderson 9-species, 19-reaction chemistry mechanism[12] solved with a finite-rate kinetics scheme and a constant-pressure combustion model.

Results

The purpose of this paper is to present results on two different aspects of the model. The first is an examination of how the computational solution is impacted when considering the presence of the nitrogen curtain purge used in the experiment to cool the optical access. Second, the selection of a turbulence model and its influence on the solution for this class of problems is investigated.

Nitrogen Curtain Purge

In many cases when an investigator models an experiment in an attempt to reproduce collected data, assumptions are made to make either the model, the calculation, or both simpler. One type of assumption often made is neglecting features added for the purpose of the experiment that might not otherwise be present. In the experiment that produced the data used for comparison in this work,[2] four windows provided optical access into the engine chamber. To protect the windows from the hot combustion gases, a cool nitrogen curtain purge flowed across the interior surface of each window.

Previous computational work designed to reproduce this data neglected the presence of the nitrogen near the walls. Some of the solutions showed significant deviation from the experimental data in the vicinity of the wall and it was suggested that those deviations were caused by omitting the nitrogen purge in the calculation.[4]

To test this hypothesis, the presence of the nitrogen and the change in the geometry created by the addition of the windows were modeled. Figure 1 shows a schematic of the computational domain. The mass flow rate of the nitrogen was 0.01 kg/s (0.022 lbm/s). Three solutions were produced, each corresponding to the window location at 1 inch, 2 inches, and 5 inches, respectively, downstream from the injectors. Because the calculations are 2-D axisymmetric, it was assumed that the windows were also axisymmetric, wrapping around the outer circumference of the chamber. Clearly this is a departure from the true geometry, and future

three-dimensional calculations will better represent the size and location of the windows. The purpose here is to determine if including the nitrogen curtain purge has any impact on the solution results.

Figure 2 shows contour plots of nitrogen concentration for each of the three cases and represent an average of time-accurate results. In Figures 2a and 2b, the nitrogen is not flowing across the window as it should. This is likely due to a combination of two effects. First, because the nitrogen flow is modeled as axisymmetric with the same mass flow rate, its injection velocity is far lower than it was in the experiment. Combined with the presence of a strong recirculation zone in the upstream corners of the chamber which pulled the low-speed nitrogen into it, the nitrogen was unable to flow as intended. A three-dimensional simulation, with the windows modeled more accurately, will result in a greater nitrogen velocity, and should change the nitrogen concentration profile in the vicinity of the recirculation zone. However, even in the three-dimensional case, nitrogen likely will still be pulled into the recirculation zone, though to a lesser degree. Thus, we can use the results here to draw qualitative conclusions as to the behavior of the actual engine. At five inches downstream from the injector, the nitrogen purge is not strongly influenced by the upstream recirculation zone, as can be seen in Figure 2c. The nitrogen flows across the window as intended and this is what will be expected from three-dimensional simulations as well.

Figures 3 and 4 show a comparison amongst the hydrogen and oxygen mole fraction profiles with and without the nitrogen purge, and the experimental data. As seen in the data in Figure 3, it is not far outside the shear layer that the hydrogen mole fraction begins to steadily drop off in the radial direction due to the presence of the nitrogen. While the effect is significant at the one inch station, it is also present at the two and five inch stations, albeit to a lesser extent. The sharp decrease in the hydrogen mole fraction at the one inch station is likely due to the nitrogen in the experiment is being pulled into the region of strong recirculation as suggested by the computation.

As shown in Figure 4, the hydrogen does not penetrate as quickly into the oxygen core when the nitrogen is present. The species mole fraction profiles are clearly impacted by the presence of the nitrogen, even near the chamber centerline. By incorporating the nitrogen into the model, the results match the data as well as or more closely than without the nitrogen. The influence of the nitrogen becomes more profound as one moves downstream since the propellants have had more time to mix.

Recall that the nitrogen is an artifact of the experimental data collection process, and as such, might often be neglected by someone trying to compare numerical results to experiment. The results here suggest that when comparing to experimental data, one should be mindful in how any neglected experimental features might impact computational results were they included in the simulation. This is especially important when using numerical results to validate flow models. Discrepancies with the data could be misinterpreted as an inadequacy in a model when in fact the discrepancies may be caused by improperly setting up the simulation. Likewise, the experimenter should be mindful when drawing conclusions from such an experiment and extrapolating them to actual application hardware where experimental features like a nitrogen curtain purge may not be present.

Turbulence Models

When modeling this class of flows, it is necessary to choose a turbulence model. Which model and its impact on the solution are the focus of this section. Results were obtained four times with differing turbulence models. The four models are a realizable k-epsilon, cubic k-epsilon, Goldberg R_t, and k-epsilon-R_t. Comparisons are made at the 5-inch station and include the nitrogen curtain purge. The one-inch and two-inch stations are not included in the present analysis due in part to the questionable interaction of the nitrogen flow and the recirculation region attributed to the domain geometry. Comparisons of the turbulence models may be revisited in conjunction with three-dimensional calculations at the other two measuring stations.

Figure 5 shows the various profiles for hydrogen mole fraction. Each profile predicts that the hydrogen diffuses into the oxygen core more rapidly than does the experiment. The linear k-epsilon model seems to best represent the data, over-predicting the mixing rate the least, and best matching the slope of the data. A similar conclusion is drawn from Figure 6, showing the oxygen mole fraction. The results show the oxygen diffusing into the hydrogen more rapidly than occurred in the experiment. Again, the linear k-epsilon model seems to best represent the data.

One of the reasons that these models are over-predicting the mixing rate may be that they are best suited to steady flows. The present flow, however, is not steady. The shear layer in this flow oscillates, resulting in an unsteady flame. The solutions in the figures are averages of several time-accurate solutions. This average has been found to be different than a solution to a "quasi-steady" calculation and better predicted the data in many cases.[5] Because it is fundamentally more prudent to compare the experiment to averaged time-accurate solutions rather than "quasi-steady" solutions, and because the time-accurate averages tend to match the data better in most other investigated cases for this problem, comparisons to the averaged time-accurate results are made here. Further

study is required to determine if "quasi-steady" results, utilizing turbulence models suited to that type of calculation, would provide different conclusions than those presented here.

Another thought to consider is the fact that the experimental hardware is not axisymmetric. The actual chamber cross-section is square and the nitrogen purge only exists on the top and bottom of the chamber. Further, turbulence is inherently three-dimensional. The turbulence models may be insufficient to predict turbulent structure of this flow. Thus, the fact that the linear k-epsilon model best represents the data, despite the fact that one might expect some of the other models to do a better job, may be an artifact of the axisymmetric nature of the modeled geometry and the implied assumption of isotropic turbulence. Three-dimensional computations are needed to investigate this possibility further.

Figure 7 shows the mean axial velocity profiles. While the k-epsilon model again does the best at predicting the experimental data, each solution continues to show evidence of the shear layer which is not indicated in the data. By the time the flow reaches the five inch station, the experiment shows that the momenta of the two jets have fully diffused, leaving the characteristics of only a single jet. However, the computational results continue to show evidence of the velocity peaks of the hydrogen gas. Again, this may be attributable to the fact that the k-epsilon and R_t turbulence models are suited to isotropic flows more steady than the present shear flow.

Lastly, Figure 8 provides profiles of temperature. This simply shows a comparison of the results when using the different turbulence models. No conclusions can be drawn as to the best turbulence model for temperature as no experimental data is currently available, however the figure does serve to illustrate the sensitivity of the flow temperature on the turbulence model.

Though it can be concluded from Figures 5 – 7 that the linear k-epsilon model best represents the experimental data, it is not the intent here to suggest any given turbulence model is best suited to this class of problems. As previously suggested, the results may be biased by the fact that the geometry is being modeled as axisymmetric and that the turbulence is truly three-dimensional in nature. The primary point is to show that the selection of a turbulence model for reacting, shear, coaxial flows does impact on the solution. The only conclusion that can be drawn from the figures presented here is that the k-epsilon model is the best model *of those investigated thus far*. One has only to review the literature to find numerous other turbulence models that may do better at representing the data in this type of problem.

CFD++ has a LNS (Limited Numerical Scales) turbulence model which is a hybrid between RANS and LES approaches.[13] This model is designed to modify the stress tensor by applying an LES formulation in regions of unsteadiness. The effect is to reduce the eddy viscosity in these regions which will then suppress the mixing rate. The model is best suited to flows where the turbulence is assumed to be three-dimensional (i.e. vortex stretching and non-isotropic turbulence are present). Thus, the model will be examined in conjunction with future three-dimensional simulations and may provide a better means of predicting the flow characteristics.

Summary and Conclusions

Calculations were performed on a single-element, gas/gas, H_2/O_2 combustion engine as part of an ongoing effort to develop a computational methodology to be used to predict rocket engine flow fields. Using the CFD++ flow solver, two aspects of the flow were examined. It has been shown that the nitrogen curtain purge used to cool the optical access windows in the experiment impacted the experimental and computational data. When included in the computational model, the presence of the nitrogen significantly influences the results. This suggests that both the experimenter and the modeler should be mindful when interpreting results of an experiment or simulation when all the physical features of a particular problem are not considered.

The impact of the turbulence model on the solution to shear, coaxial flows was also investigated. Of the models examined, it was shown that the realizable k-epsilon model produces the best representation of the experimental data. This conclusion is tempered, however, by the fact that RANS turbulence models are best suited to steady flows and the present turbulent, coaxial shear layer is inherently unsteady. The hybrid LNS turbulence model may fundamentally be the best model to apply to this class of problems, and will be investigated in the future.

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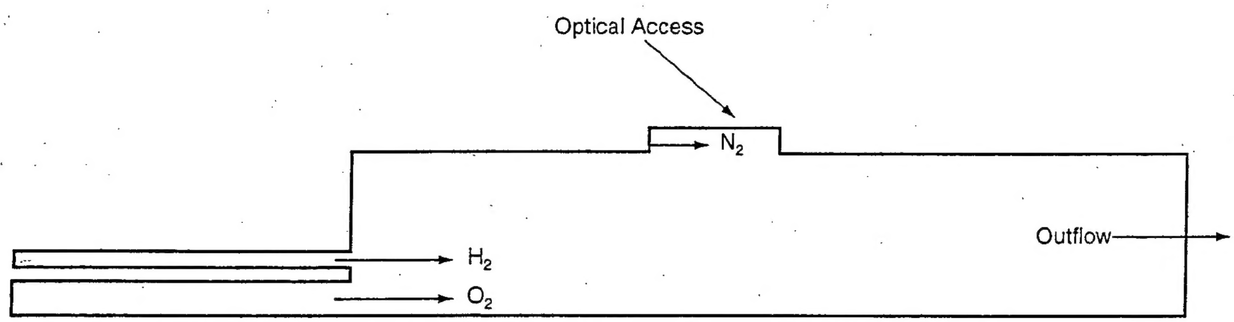

Figure 1. Schematic of computational domain.

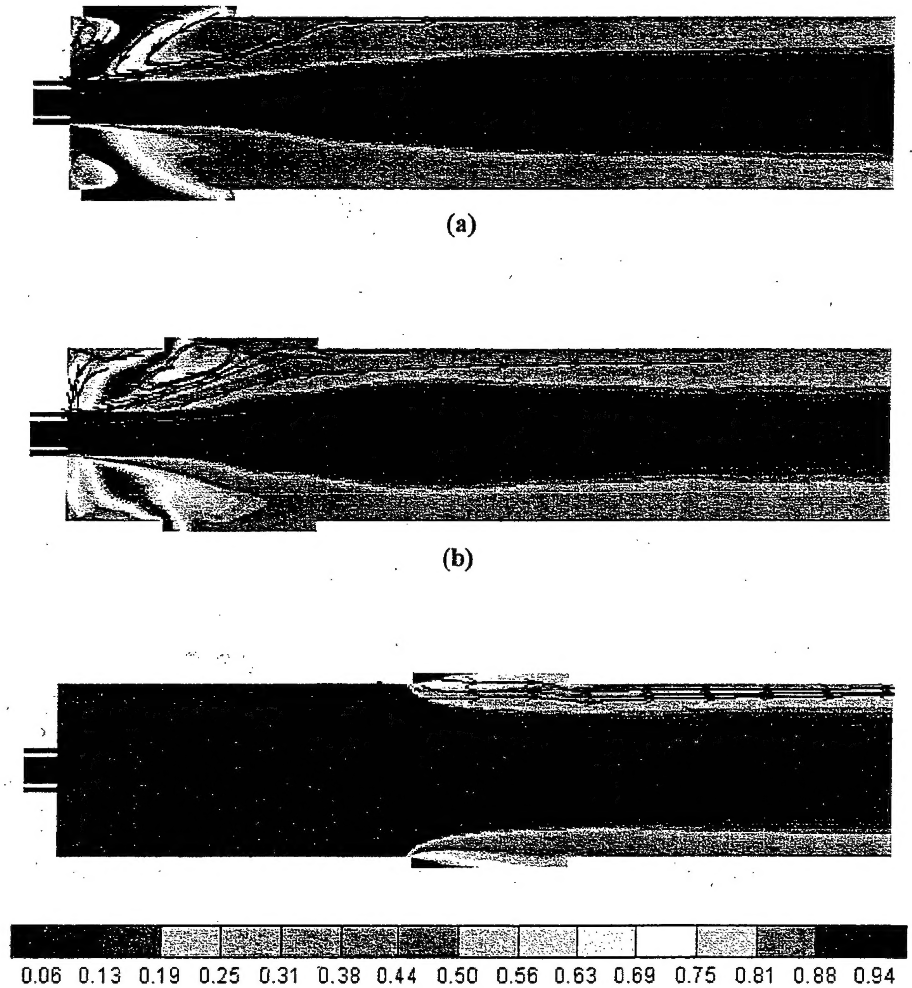

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Figure 2. Contours of N_2 concentration. N_2 injected at (a) 1 inch, (b) 2 inches, and (c) 5 inches downstream from injectors.

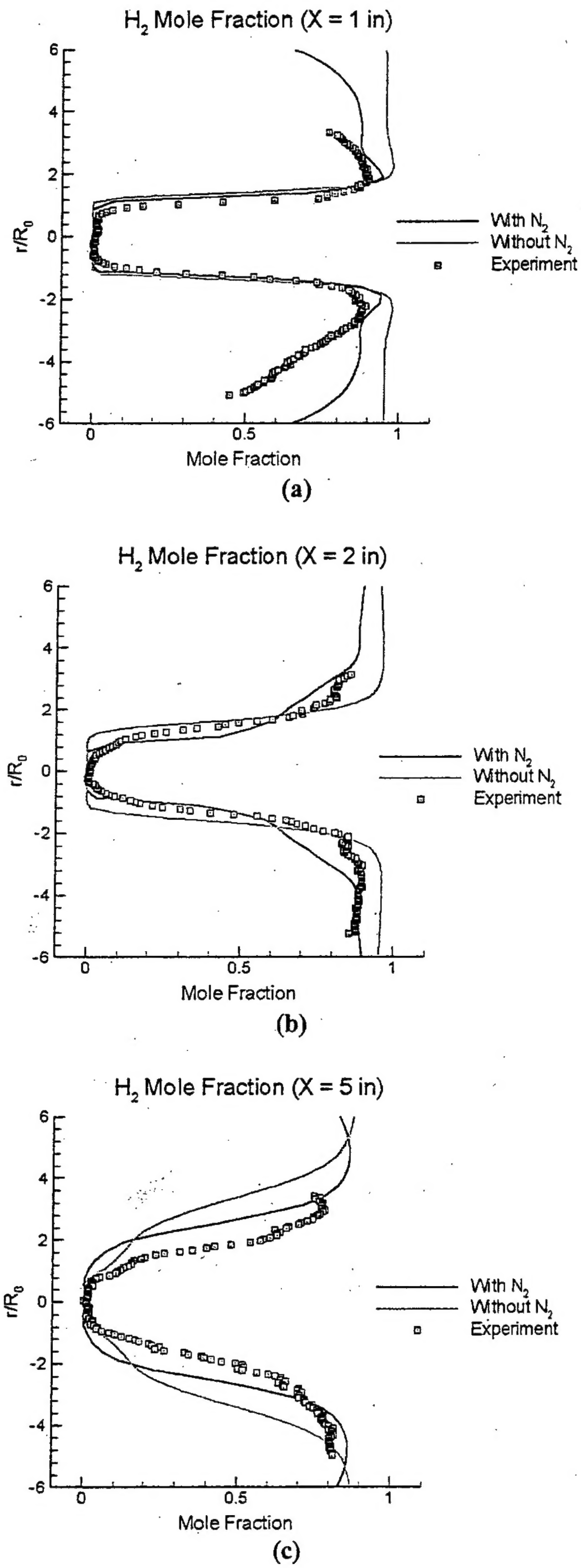

Figure 3. Hydrogen mole fraction profiles showing influence of N_2 at (a) 1 inch, (b) 2 inches, and (c) 5 inches downstream of injectors.

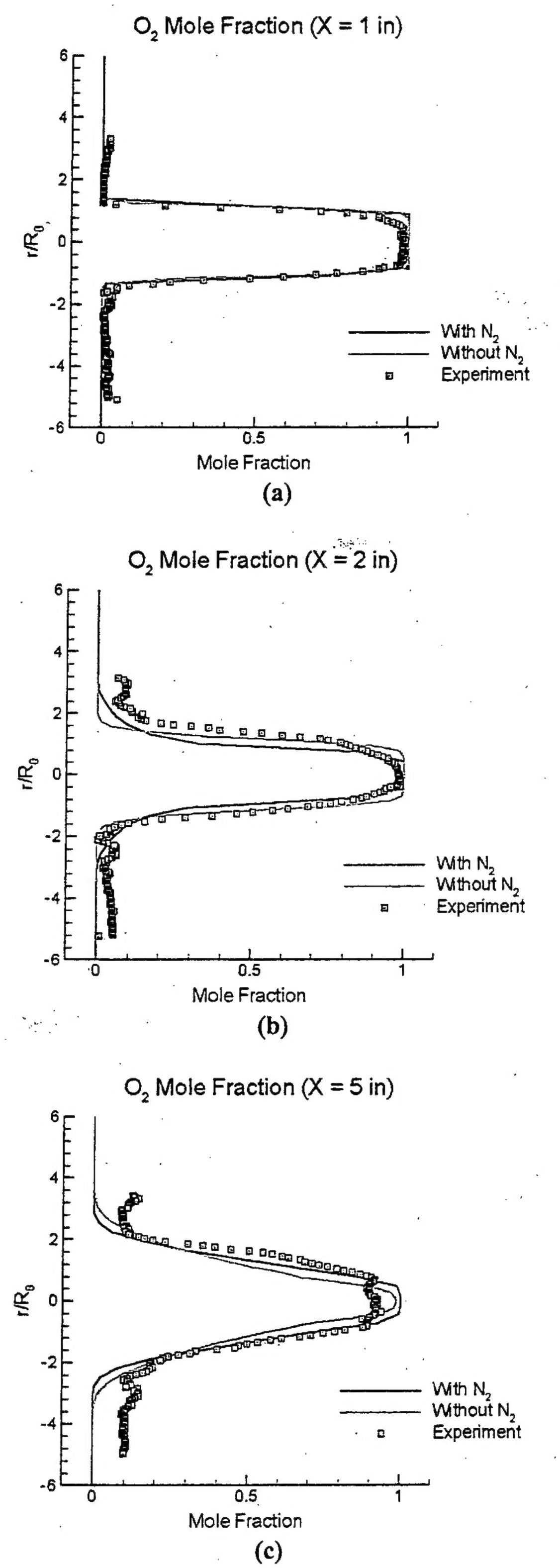

Figure 4. Oxygen mole fraction profiles showing influence of N_2 at (a) 1 inch, (b) 2 inches, and (c) 5 inches downstream of injectors.

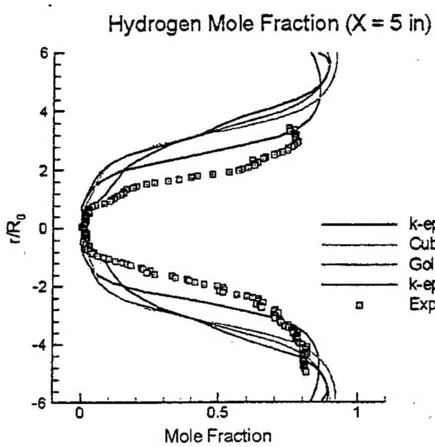

Figure 5. Hydrogen mole fraction profiles showing influence of turbulence model selection.

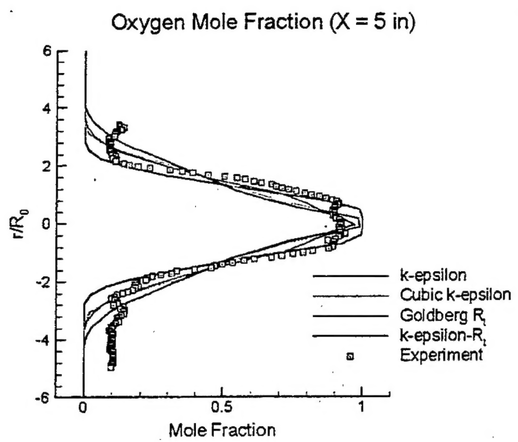

Figure 6. Oxygen mole fraction profiles showing influence of turbulence model selection.

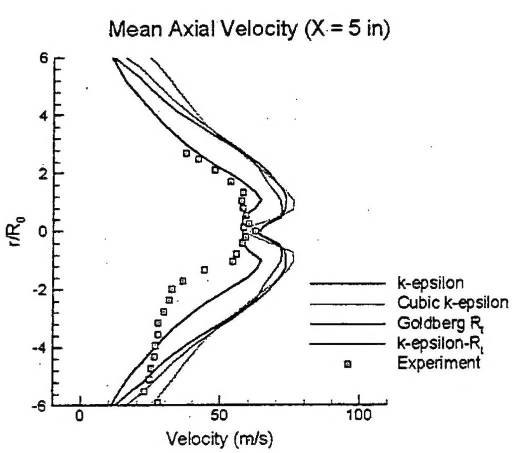

Figure 7. Mean axial velocity profiles showing influence of turbulence model selection.

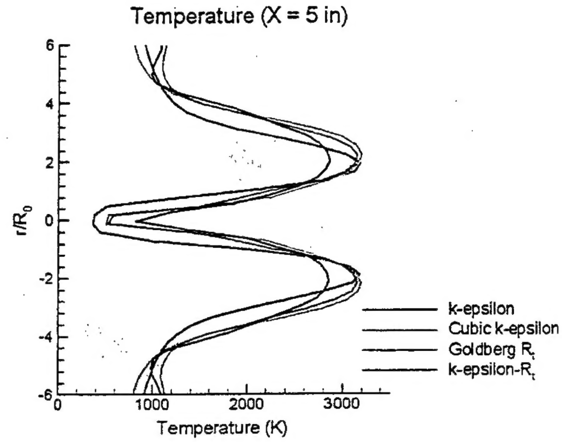

Figure 8. Temperature profiles showing the influence of the turbulence model selection.